Chemical Hydrogen Storage: Control of H_2 Release from Ammonia Borane

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EERE Program Review 5/24/04

(*This presentation does not contain any proprietary or confidential information*)

Objectives

- **Hypothesis:** Nano phase hydrogen storage materials will have different thermodynamic and kinetic properties compared to bulk hydrogen storage materials.

- **Nano particles of Hydrogen Storage material**
  - Control Reactivity (enhanced rate of H_2 release)
  - Control Selectivity (prevent Borazine formation)
  - Can we prevent fusion of the nanoparticles as the reaction proceeds? (Don't want to lose nano properties)

- **Use Mesoporous Scaffolds**

Technical Barriers and Targets

On-board hydrogen storage for FC vehicles

Volumetric Density

year	2010	2015
KWh/liter	1.5	2.7
MJ/liter	5.4	9.7
gm/liter	45	81

Gravimetric Density

year	2010	2015
KWh/kg	2	3
MJ/kg	7.2	10.8
gm/kg	60	90

Operational temperature: -20 < ˚C < 80

Material with 9 wt% H_2 that releases H_2 < 80˚ C

Approach: Nanophase BNH compounds

NH_xBH_x: Stores significant quantity of hydrogen (6 wt%/step)

	Wt% H_2	T (°C)
$NH_4BH_4 \rightarrow NH_3BH_3 + H_2$	6.1	<25
$NH_3BH_3 \rightarrow NH_2BH_2 + H_2$	6.5	<120
$NH_2BH_2 \rightarrow NHBH + H_2$	6.9	>120
$NHBH \rightarrow BN + H_2$	7.3	>500

How does NH_3BH_3 embedded in a mesoporous scaffold compare to bulk NH_3BH_3?

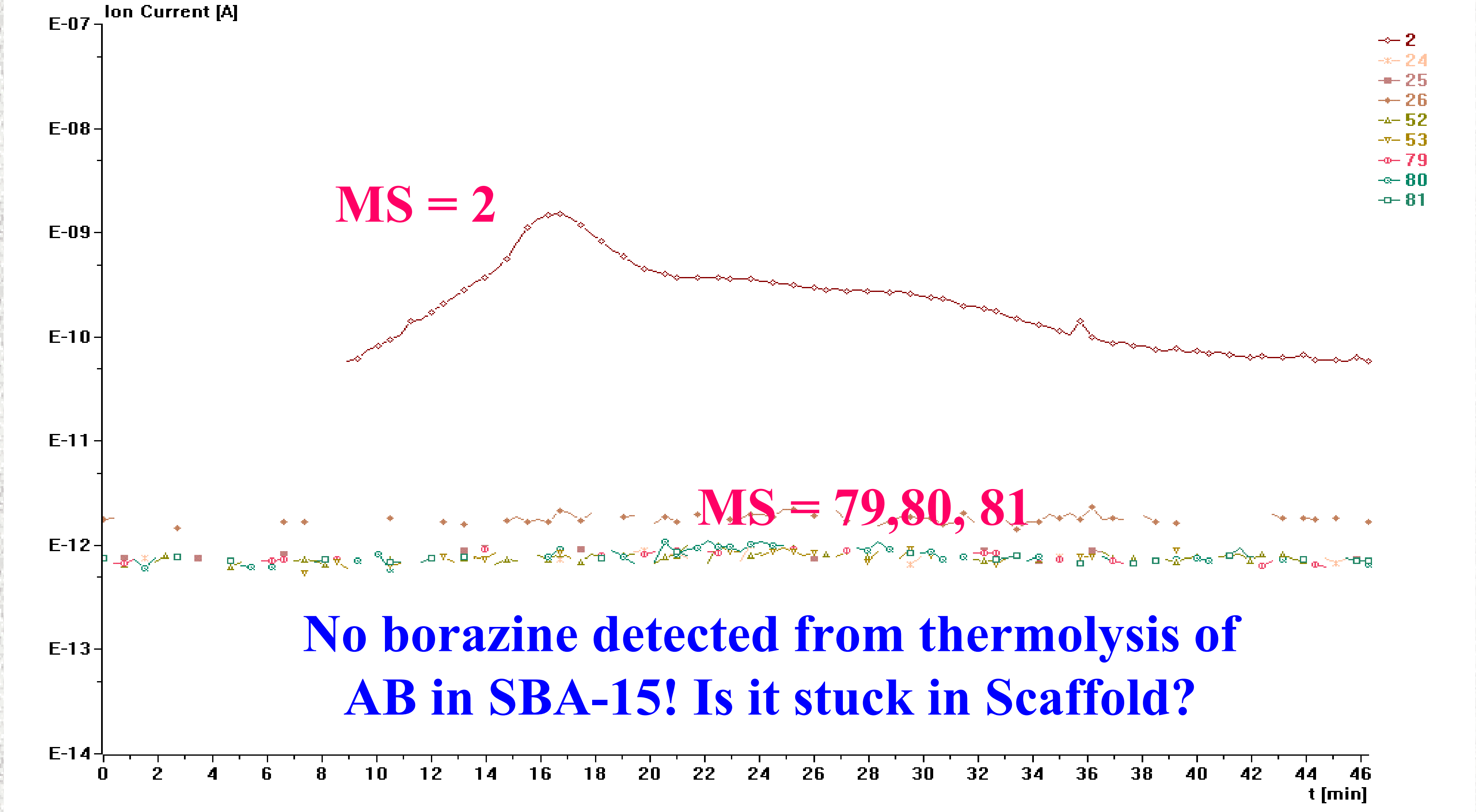
- Minimize Borazine formation?
- Change Thermochemistry?
- Change kinetics?

- TEM/BET/EDX
  - Material Characterization (Surface area, porosity)
- DSC/MS (differential scanning calorimetry/mass spec)
  - Volatile products
  - Thermodynamics
  - Kinetics
- Solid State NMR ^{11}B
  - Product identity
  - Kinetics

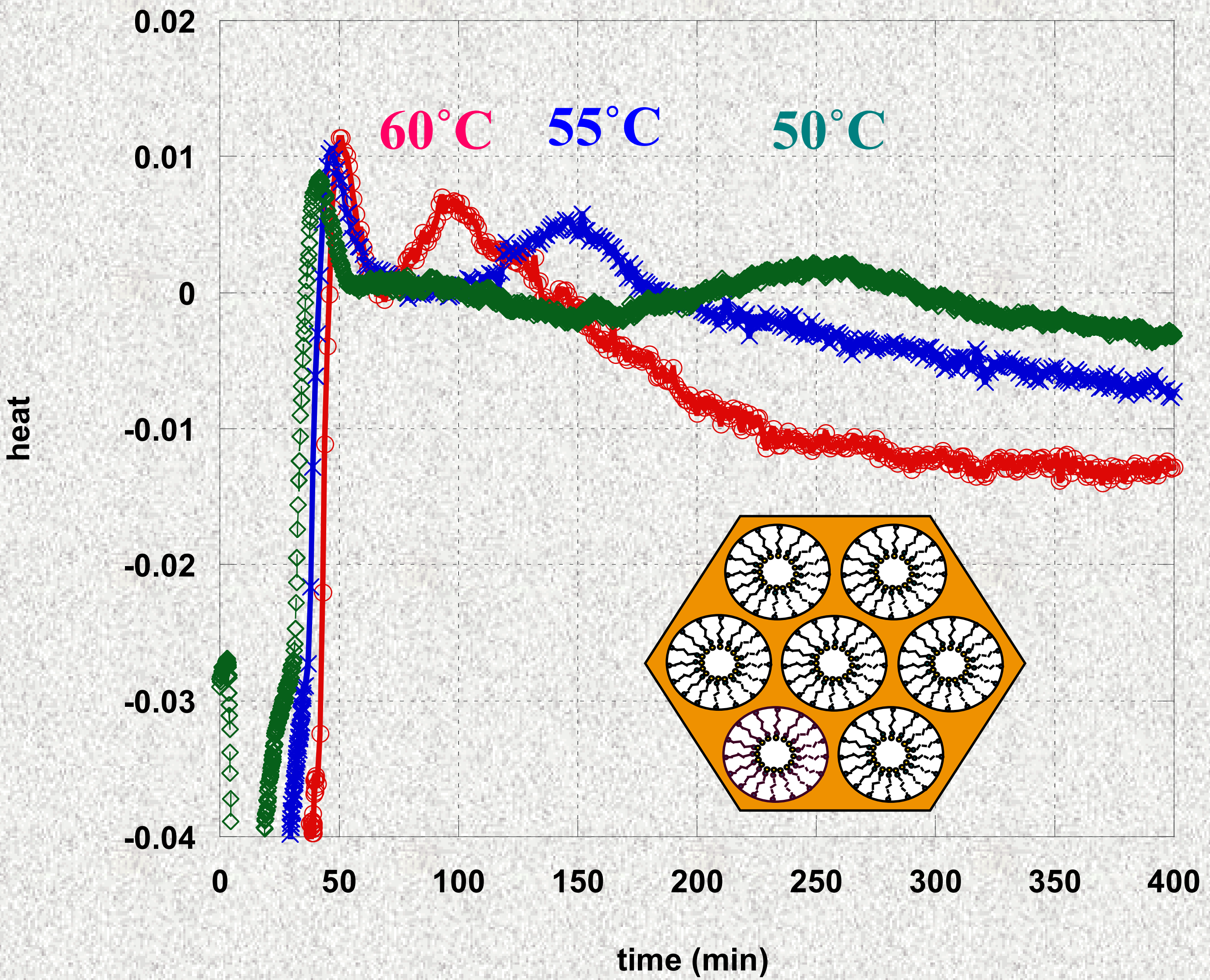
Project Safety

- Use safe handling procedures as outlined by MSDS
- In experiments where hydrogen is released, large quantities of inert gas are used to avoid any build up in concentration of hydrogen.
- Materials are treated with dilute acid at conclusion of experiments to destroy any residual hydrogen.

Volatile Products from NH_3BH_3 in Mesoporous scaffold

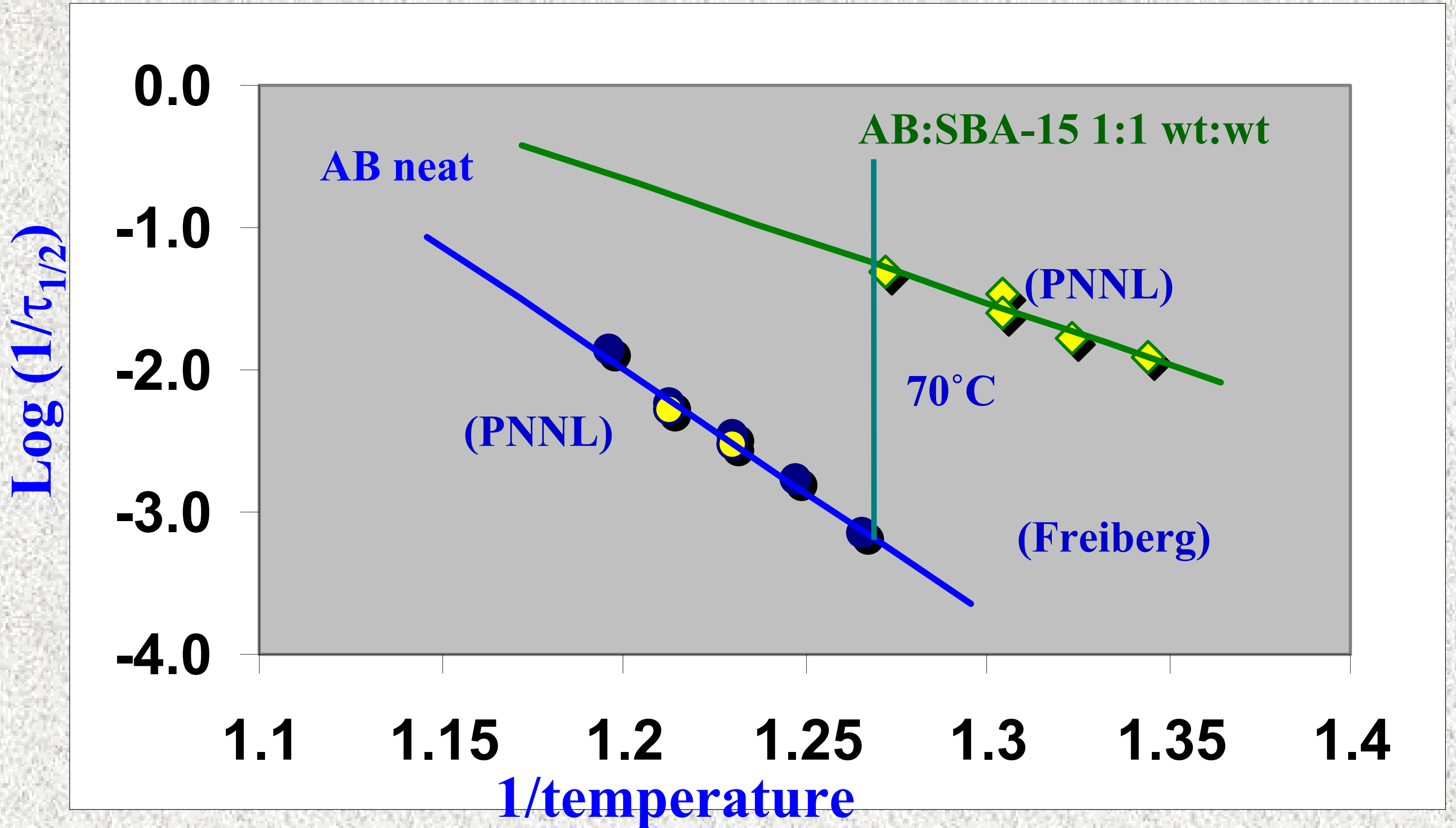


Increase the Temperature Increase the rate of H_2 release

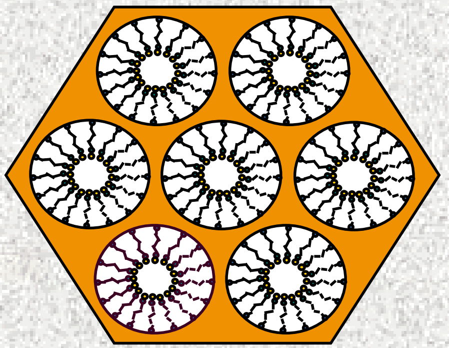


Ammonia borane in SBA-15

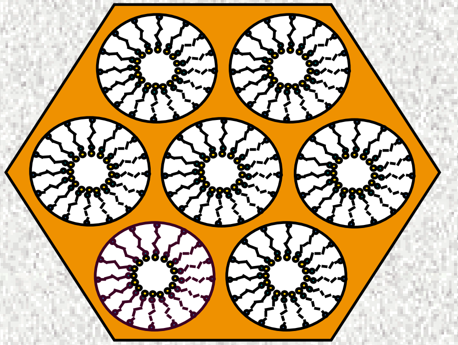
Comparison of H_2 Release: AB versus mesoporous AB



Rate of hydrogen release is 1 to 2 orders of magnitude faster with mesoporous scaffold



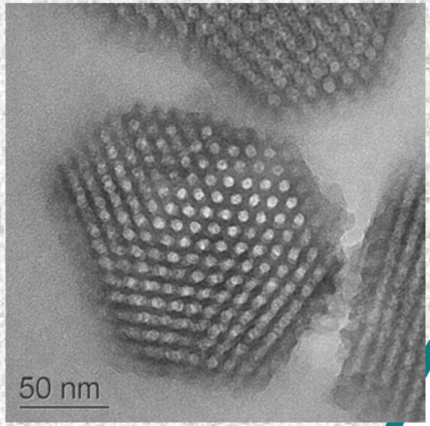
Summary

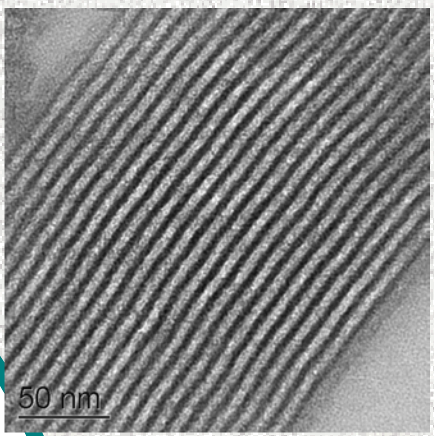


►H_2 release from NH_3BH_3 in Mesoporous scaffolds:

- *Control* of selectivity of H_2 release from AB
  - SBA-15 appears to guide NH_3BH_3 towards linear polymer formation.
  - No borazine seen in volatile products or left behind in scaffold.
  - No cyclized products observed in NMR and DSC data show process is less exothermic
- *Control* of reactivity for H_2 release from AB
  - 1-2 orders of magnitude faster!

Future Efforts





65 Å

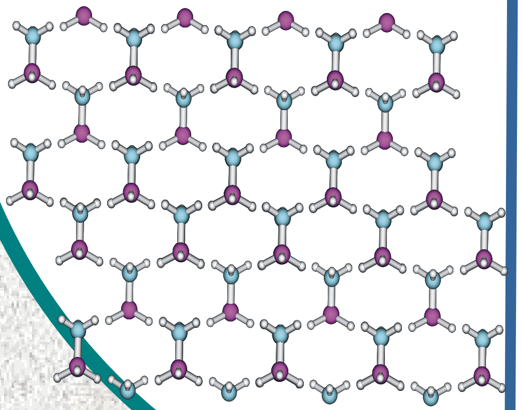
Vary pore diameter 60-300 nm

Coat nano particles (in vs. out)

Thin films (curvature)

Cover Si-OH (alkane)

More detailed kinetic studies



Surface interactions?

Radius of curvature?

Collaborators

- Y Shin, S Li SBA-15
- C Wang TEM
- J Coleman SEM
- D Matson Synthesis
- J Fulton, Y Chen XAFS
- S Addleman G Fryxell Mesos
- S Smith, B Kay Kinetics
- W Shaw, C Yonker NMR
- R Williford Modeling
- V Viswanathan Fuel Cells
- G Whyatt Systems Eng
- K Peterson Hi Pressure
- N Baer purification
- J Franz, D Camaioni, D Schubert, L Sneddon, T Baker Chemistry

Acknowledgement

PNNL FY04 NanoScience & Technology Initiative